

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081523\
 Data File : VV031809.D
 Acq On : 15 Aug 2023 14:27
 Operator : SY/MD
 Sample : 03965-06ME
 Misc : 5.37g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A48H2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

Signal : TIC: VV031809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.275	67	73	92	rVB	114685	174309	11.14%	1.356%
2	1.503	109	144	149	rBV3	115407	338217	21.62%	2.632%
3	2.037	300	310	326	rBV	321231	470816	30.09%	3.664%
4	2.381	410	417	428	rVB	40815	64003	4.09%	0.498%
5	2.500	447	454	461	rVB4	10379	15225	0.97%	0.118%
6	2.561	464	473	486	rVB2	14247	30804	1.97%	0.240%
7	2.831	555	557	561	rBV5	1607	1160	0.07%	0.009%
8	2.928	585	587	591	rVV4	1337	948	0.06%	0.007%
9	3.079	630	634	637	rBV4	1770	1470	0.09%	0.011%
10	3.146	652	655	657	rBV3	1467	985	0.06%	0.008%
11	3.272	691	694	696	rBV2	928	732	0.05%	0.006%
12	3.333	710	713	716	rBV5	1573	1290	0.08%	0.010%
13	3.442	742	747	751	rBV6	1968	1758	0.11%	0.014%
14	3.503	764	766	771	rVB5	1577	1322	0.08%	0.010%
15	3.535	774	776	779	rBV	1261	766	0.05%	0.006%
16	3.574	785	788	793	rVB7	1232	870	0.06%	0.007%
17	3.654	807	813	815	rBV7	1952	2313	0.15%	0.018%
18	3.744	838	841	845	rBV5	1497	1256	0.08%	0.010%
19	3.802	848	859	895	rBV2	118548	420483	26.88%	3.272%
20	4.249	983	998	1027	rVV	273287	731653	46.77%	5.694%
21	4.452	1059	1061	1063	rBV3	1642	737	0.05%	0.006%
22	4.548	1088	1091	1095	rBV5	1787	1340	0.09%	0.010%
23	4.568	1095	1097	1101	rVV4	1636	1414	0.09%	0.011%
24	4.741	1148	1151	1152	rBV2	2082	1217	0.08%	0.009%
25	4.809	1169	1172	1177	rVB7	1486	1149	0.07%	0.009%
26	4.831	1177	1179	1182	rBV4	1198	775	0.05%	0.006%
27	4.957	1201	1218	1249	rBV2	604645	1564468	100.00%	12.174%
28	5.304	1322	1326	1328	rBV4	1229	990	0.06%	0.008%
29	5.413	1356	1360	1363	rBV6	1700	1282	0.08%	0.010%
30	5.432	1363	1366	1367	rBV2	2139	921	0.06%	0.007%
31	5.474	1376	1379	1381	rBV3	1215	899	0.06%	0.007%
32	5.539	1386	1399	1425	rBV	426788	938539	59.99%	7.303%
33	5.828	1471	1489	1509	rBV2	48402	115914	7.41%	0.902%
34	5.992	1526	1540	1568	rBV	369614	801978	51.26%	6.241%
35	6.281	1628	1630	1633	rBV3	1462	930	0.06%	0.007%
36	6.333	1644	1646	1649	rVB3	1918	1059	0.07%	0.008%

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 Title : VOC Analysis

37	6.458	1683	1685	1689	rBV5	1452	1144	0.07%	0.009%
38	6.545	1709	1712	1715	rBV5	1553	1346	0.09%	0.010%
39	6.686	1754	1756	1759	rVB4	1690	846	0.05%	0.007%
40	6.821	1796	1798	1803	rVB6	1513	1144	0.07%	0.009%
41	6.854	1804	1808	1812	rBV5	1788	1384	0.09%	0.011%
42	6.918	1818	1828	1847	rBV	157812	315507	20.17%	2.455%
43	7.207	1916	1918	1920	rBV3	1440	719	0.05%	0.006%
44	7.249	1920	1931	1955	rVV	513362	957366	61.19%	7.450%
45	7.497	2004	2008	2011	rBV5	2767	2245	0.14%	0.017%
46	7.561	2019	2028	2046	rBV2	111508	226057	14.45%	1.759%
47	7.738	2079	2083	2086	rBV6	1907	1680	0.11%	0.013%
48	7.982	2156	2159	2163	rBV4	1669	1512	0.10%	0.012%
49	8.047	2167	2179	2211	rBV	375974	946650	60.51%	7.367%
50	8.532	2327	2330	2334	rBV4	1480	1292	0.08%	0.010%
51	8.712	2380	2386	2388	rBV5	1421	1244	0.08%	0.010%
52	8.792	2399	2411	2440	rBV	694445	1219861	77.97%	9.493%
53	8.979	2466	2469	2472	rBV5	1754	1262	0.08%	0.010%
54	9.140	2517	2519	2524	rBV5	1702	1550	0.10%	0.012%
55	9.207	2537	2540	2543	rVV5	1460	982	0.06%	0.008%
56	9.227	2543	2546	2551	rVB6	1482	1520	0.10%	0.012%
57	9.349	2579	2584	2587	rBV7	1699	1584	0.10%	0.012%
58	9.368	2587	2590	2594	rVV6	1629	1389	0.09%	0.011%
59	9.474	2621	2623	2625	rBV2	1054	717	0.05%	0.006%
60	9.638	2672	2674	2679	rVB5	1524	999	0.06%	0.008%
61	9.686	2686	2689	2693	rVB5	1433	1042	0.07%	0.008%
62	9.715	2696	2698	2699	rBV2	1821	834	0.05%	0.006%
63	9.796	2719	2723	2726	rBV6	1222	1138	0.07%	0.009%
64	9.899	2748	2755	2757	rBV8	2321	2825	0.18%	0.022%
65	9.982	2778	2781	2787	rBV6	1798	1348	0.09%	0.010%
66	10.162	2825	2837	2858	rBV	590097	959122	61.31%	7.464%
67	10.333	2883	2890	2896	rBV8	4387	5259	0.34%	0.041%
68	10.484	2934	2937	2939	rBV4	2143	1479	0.09%	0.012%
69	10.696	3001	3003	3008	rVB2	1137	767	0.05%	0.006%
70	10.821	3040	3042	3046	rBV4	1588	1133	0.07%	0.009%
71	10.860	3050	3054	3055	rBV4	2074	1227	0.08%	0.010%
72	11.088	3123	3125	3129	rVB5	1391	915	0.06%	0.007%
73	11.127	3134	3137	3140	rBV3	1149	940	0.06%	0.007%
74	11.194	3146	3158	3178	rBV	753243	1200008	76.70%	9.338%
75	11.567	3262	3274	3293	rBV	749428	1172065	74.92%	9.121%
76	11.734	3325	3326	3330	rBV4	1800	1150	0.07%	0.009%

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 ClientSampleId :
 A48H2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

77	11.966	3394	3398	3399	rBV4	1702	946	0.06%	0.007%
78	12.175	3460	3463	3465	rBV4	1294	853	0.05%	0.007%
79	12.201	3465	3471	3477	rVB7	4627	6211	0.40%	0.048%
80	12.329	3500	3511	3518	rBV9	8133	15313	0.98%	0.119%
81	12.429	3539	3542	3545	rBV5	1891	1473	0.09%	0.011%
82	12.455	3548	3550	3554	rBV5	1607	1326	0.08%	0.010%
83	12.529	3570	3573	3574	rBV3	1939	1253	0.08%	0.010%
84	12.683	3612	3621	3623	rBV7	1831	2838	0.18%	0.022%
85	12.747	3638	3641	3644	rVB3	1485	939	0.06%	0.007%
86	13.050	3732	3735	3737	rBV4	1418	919	0.06%	0.007%
87	13.217	3785	3787	3790	rVB4	1814	792	0.05%	0.006%
88	13.236	3790	3793	3795	rVB4	1946	844	0.05%	0.007%
89	13.381	3833	3838	3839	rBV4	4034	3220	0.21%	0.025%
90	13.509	3874	3878	3881	rBV6	1681	1840	0.12%	0.014%
91	13.612	3907	3910	3911	rBV3	1353	841	0.05%	0.007%
92	13.972	4019	4022	4023	rBV3	1964	1238	0.08%	0.010%
93	14.069	4050	4052	4056	rVB5	1916	1109	0.07%	0.009%
94	14.088	4056	4058	4061	rBV4	1561	1008	0.06%	0.008%
95	14.365	4136	4144	4156	rBV	42312	64513	4.12%	0.502%
96	14.596	4212	4216	4221	rBV6	1736	2305	0.15%	0.018%
97	14.670	4234	4239	4242	rBV5	2039	2062	0.13%	0.016%
98	14.966	4327	4331	4332	rBV3	1599	1052	0.07%	0.008%
99	15.075	4363	4365	4367	rBV2	1491	869	0.06%	0.007%
100	15.111	4372	4376	4377	rBV3	2108	1548	0.10%	0.012%

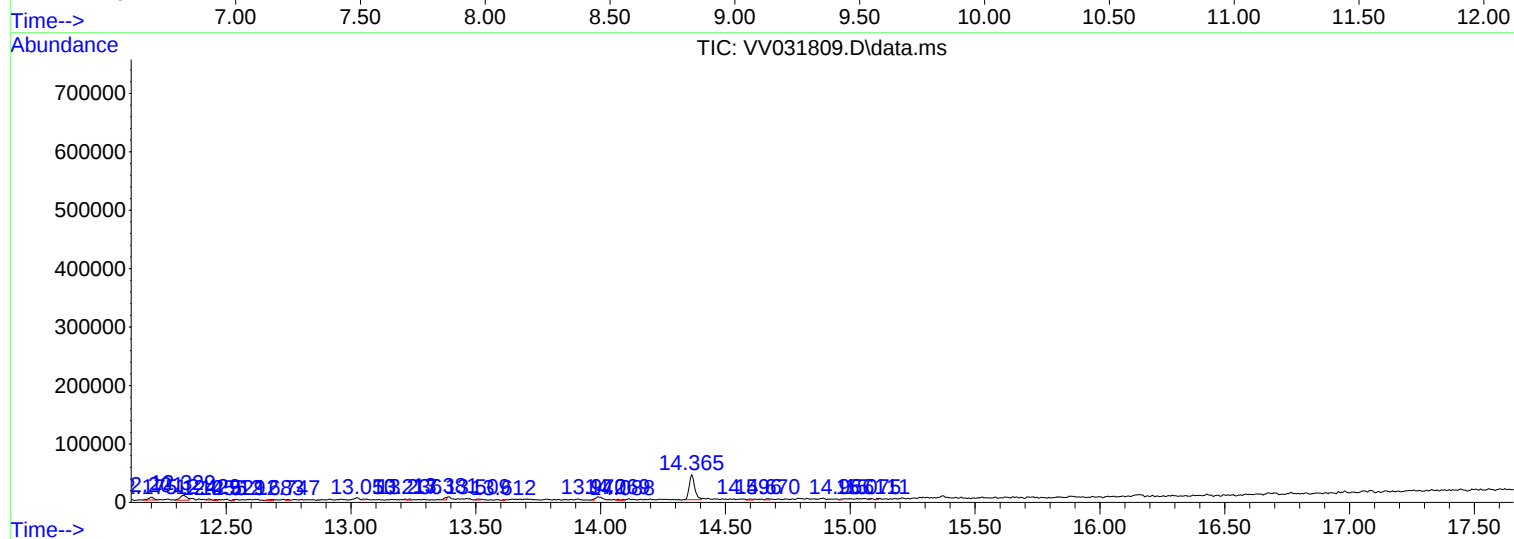
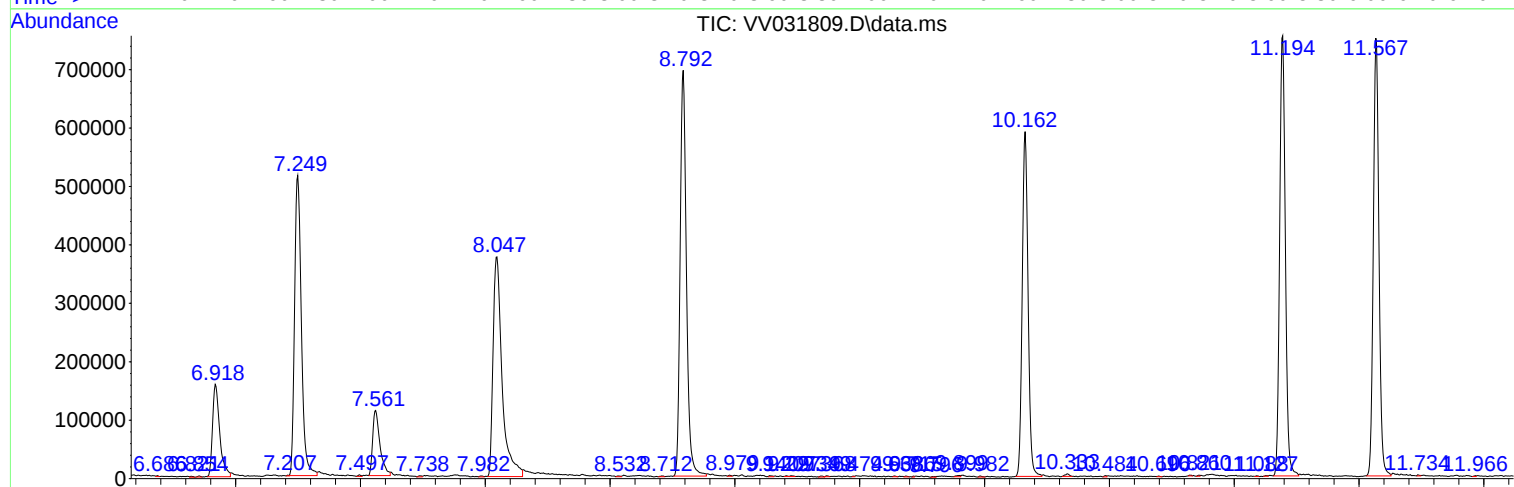
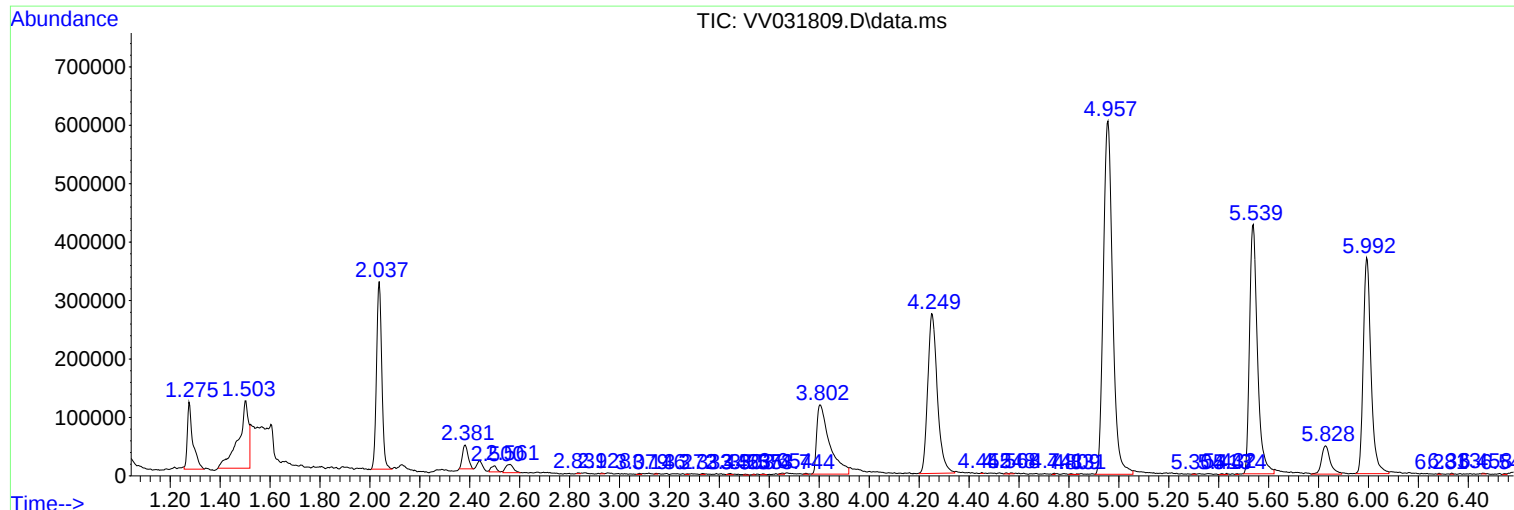
Sum of corrected areas: 12850556

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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
A48H2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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A48H2ME

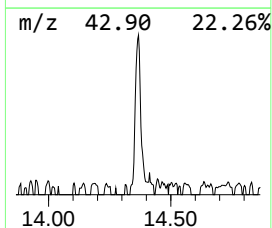
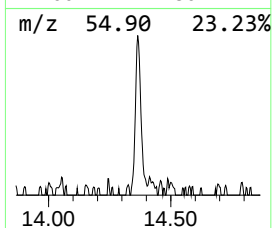
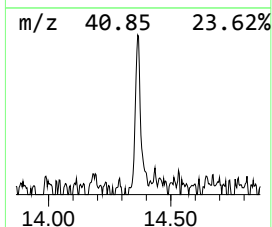
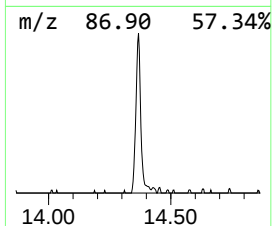
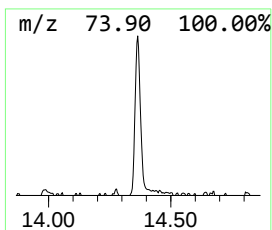
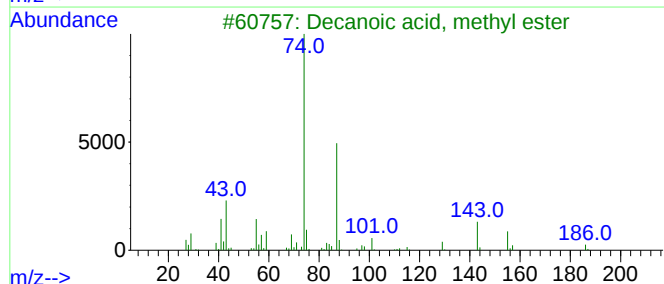
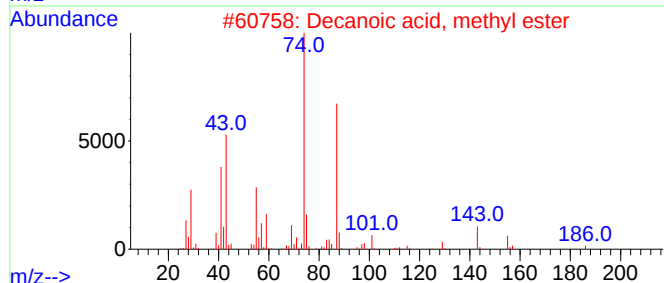
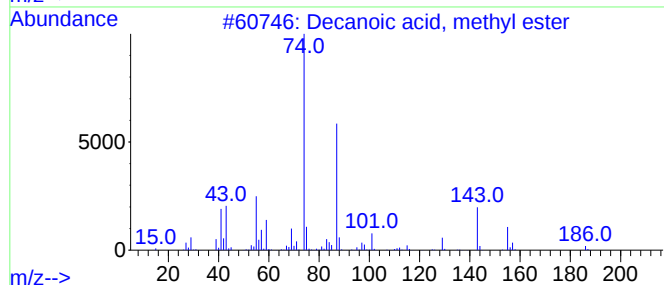
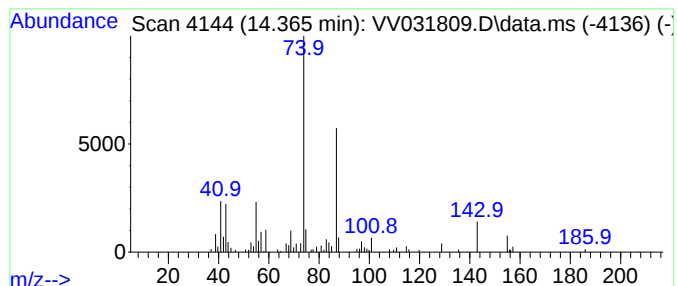
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Decanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.365	2.69 ug/L	64513	1,4-Dichlorobenzene-d4	11.194

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	96
2			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	92
3			Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	91
4			Methyl 8-methyl-nonanoate	186	C11H22O2	1000452-00-9	90
5			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Decanoic acid, ...	14.365	2.7	ug/L	64513	3	11.194	1200010	50.0